INL/CON-08-14245
PREPRINT

Coupled High Fidelity Thermal Hydraulics and Neutronics for Reactor Safety Simulations

International Conference on Reactor Physics, Nuclear Power: A Sustainable Resource

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September 2008

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Abstract

This work is a continuation of previous work on the importance of accuracy in the simulation of nuclear reactor safety transients. Although qualitative in nature, future work will be more quantitative. The focus will be on the study of a simplified single phase nuclear reactor primary system. The transient of interest, Unprotected Loss of Flow (ULOF), will be investigated to determine the importance of accuracy related to passive (inherent) safety systems. For the ULOF transient, the coolant pump is turned off and the un'SCRAM'ed reactor transitions from forced convection to natural circulation. Results will be presented that show the difference that the first order in time truncation physics makes on the transient. The purpose of this document is to illuminate possible problems in traditional reactor simulation approaches. Detailed studies need to be done on each simulation code for each transient analyzed to determine if the first order truncation physics plays an important role.

1. Introduction

This work is a continuation of previous work on the investigation of the impact of first order truncation physics on nuclear reactor safety transients (Pope and Mousseau, 2007, Mousseau 2007, Mousseau 2006, Mousseau 2005, Mousseau 2004). Although there is a large amount of work done on verification and validation for neutronics, and some work done on validation of thermal hydraulics there is almost no work done on verification or validation of coupled code calculations.

There are a variety of errors that impact the physics of a simulation of a system that includes neutron diffusion, thermal conduction, and thermal hydraulics. There are model errors and input errors that affect the accuracy of all of the component physics. This is related to the validation of the components and the validation of the system of components. Such work is out side of the scope of this manuscript. This paper will focus on the verification of the system calculation and its components. To be clear, verification is demonstrating that the models are solved accurately (the focus of this paper) and validation is the demonstration that the model chosen represents reality (this work is left for later).

For verification one must both consider temporal error and spatial error. For this manuscript spatial error will be ignored and the focus will be on temporal error. Temporal error consists of two modes inter component and intra component or coupling error. Often the temporal accuracy is quantified component by component but this is only part of the problem. There are also temporal error associated with how components are coupled together to construct the solution to the system.

The rest of the manuscript will have the following structure. The second section will

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describe the simplified reactor model for this study. The third section will derive some of the truncation physics and discuss how it impacts the solution. The fourth section will show results from an unprotected loss of flow transient and the final section will give conclusions and future work.

2. Mathematical Model

The simplified model is shown in schematic form in Figure 1. The system consists of a simple primary loop of 1-D single phase flow. The core includes the fuel and the clad and is modelled with 2-D neutron diffusion and 2-D thermal conduction. The core and the coolant exchange energy through convective heat transfer. The heat exchanger is simply modelled as a constant heat removal rate from the coolant as it flows through the downward part of the loop. The pump, located at the center of bottom of the loop, is modelled as a simple momentum source. The neutron cross sections depend on the temperature of the fuel and the density of the coolant. So the neutron flux depends on the temperature of the fuel, the temperature of the fuel depends on the heat transfer with the coolant. This results in a tightly coupled nonlinear system.

There are a few observations to be made about accuracy in this system and the ULOF transient. In this model the coolant is a closed loop. Therefore any error made in the fluid flow calculation accumulates; this is similar to transients in passive safety systems. Second, once the pump is turned off, the flow has to transition from forced convection to natural circulation. This is another property of passive cooling systems. Finally since the reactor is not SCRAM'ed there is feedback between the neutron diffusion, the thermal conduction and the coolant flow again similar to a passive safety system.

The mathematical model is broken into three parts; fluid, conduction and neutronics. The 1-D fluid flow is modelled with the following three equations that represent conservation of mass, momentum, and energy. Conservation of mass is given by,

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x} = 0 \tag{1}$$

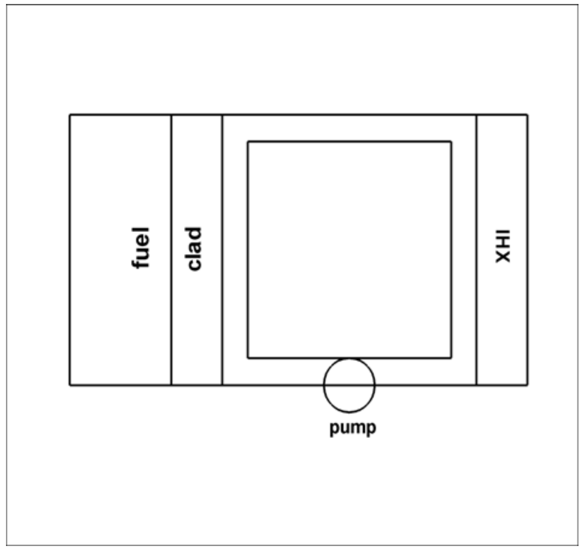

Fig. 1 Model schematic.

Here t is time, x is distance, ρ is density and v is velocity. The conservation of momentum equation is

$$\rho \frac{\partial v}{\partial t} + \rho v \frac{\partial v}{\partial x} + \frac{\partial P}{\partial x} + \rho g = - F_w \rho^2 |v| v + S_{pump} \tag{2}$$

Here the momentum equation is written in non-conservative form and P is pressure, F_w is the wall friction coefficient, and g is the acceleration due to gravity, and S_{pump} is the momentum source term only turned on in the control volume with the pump. The conservation of energy is expressed as

$$\frac{\partial \rho U}{\partial t} + \frac{\partial \rho U v}{\partial x} + P \frac{\partial v}{\partial x} = H_w (T_w - T) + S_{\sec} \tag{3}$$

Here U is the specific internal energy, H_w is the wall heat transfer coefficient which is only nonzero in the control volumes adjacent to the core (the left side of the loop in Fig. 1) T_w is the temperature of the clad, T is the temperature of the coolant and S_{sec} is the constant heat removal rate in the control volumes in the heat exchanger (the right side of the loop in fig. 1). The conservation of energy in the fuel and clad is governed by

$$\frac{\partial e_w}{\partial t} - \nabla \cdot K \nabla T = \Sigma_f e_f \phi - H_w (T_w - T) \quad (4)$$

Here ϕ is the neutron flux, K is the thermal conductivity of the fuel and clad, e_w is the energy in the wall, e_f is the energy per fission, Σ_f is the fission cross section. The fission source is only turned on in the fuel (not the clad) and the wall heat transfer only takes place in control volumes adjacent to the coolant (labelled clad in Fig. 1).

The neutronics is a single group calculation with precursors. The conservation of neutrons is given by

$$\frac{1}{v_{th}} \frac{\partial \phi}{\partial t} - \nabla \cdot D_0 \nabla \phi + \Sigma_a \phi - (1-\beta) \Sigma_f n_f \phi = \lambda C \quad (5)$$

Here v_{th} is the thermal neutron velocity, D_0 is the constant neutron diffusion coefficient, Σ_a is the absorption cross section, β is the percent of delayed neutrons, n_f is the number of neutrons generated per fission, C is the precursor concentration, and λ is the delayed neutron time constant. The precursor concentration is represented by

$$\frac{dC}{dt} - \beta \Sigma_f n_f \phi + \lambda C = 0 \quad (6)$$

The cross sections depend on the fuel temperature and coolant density by

$$\Sigma_f = \Sigma_{f0} + \frac{\partial \Sigma_f}{\partial T} (T_w - T_0) \quad (7)$$

$$\Sigma_a = \Sigma_{a0} + \frac{\partial \Sigma_f}{\partial \rho} (\rho - \rho_0) \quad (8)$$

3. Truncation Physics

To analyze the truncation physics we employ the following truncated Taylor series expansions for flux and temperature.

$$\phi^n = \phi^{n+1} - \Delta t \frac{\partial \phi}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 \phi}{\partial t^2} \quad (9)$$

$$\phi^n = \phi^{n+1/2} - \frac{\Delta t}{2} \frac{\partial \phi}{\partial t} + \frac{\Delta t^2}{8} \frac{\partial^2 \phi}{\partial t^2} - \frac{\Delta t^3}{48} \frac{\partial^3 \phi}{\partial t^3} \quad (10)$$

$$\phi^{n+1} = \phi^{n+1/2} + \frac{\Delta t}{2} \frac{\partial \phi}{\partial t} + \frac{\Delta t^2}{8} \frac{\partial^2 \phi}{\partial t^2} + \frac{\Delta t^3}{48} \frac{\partial^3 \phi}{\partial t^3} \quad (11)$$

$$T^n = T^{n+1} - \Delta t \frac{\partial T}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 T}{\partial t^2} \quad (12)$$

$$T^n = T^{n+1/2} - \frac{\Delta t}{2} \frac{\partial T}{\partial t} + \frac{\Delta t^2}{8} \frac{\partial^2 T}{\partial t^2} \quad (13)$$

$$T^{n+1} = T^{n+1/2} + \frac{\Delta t}{2} \frac{\partial T}{\partial t} + \frac{\Delta t^2}{8} \frac{\partial^2 T}{\partial t^2} \quad (14)$$

Substitution of Eq. (12), Eq. (13), and Eq. (14), into Eq. (7) yields

$$\Sigma_f^n = \Sigma_f^{n+1} - \frac{\partial \Sigma_f}{\partial T} \frac{\partial T}{\partial t} \Delta t \quad (15)$$

$$\Sigma_f^n = \Sigma_f^{n+1/2} - \frac{\partial \Sigma_f}{\partial T} \left(\frac{\partial T}{\partial t} \frac{\Delta t}{2} - \frac{\partial^2 T}{\partial t^2} \frac{\Delta t^2}{8} \right) \quad (16)$$

$$\Sigma_f^{n+1} = \Sigma_f^{n+1/2} + \frac{\partial \Sigma_f}{\partial T} \left(\frac{\partial T}{\partial t} \frac{\Delta t}{2} + \frac{\partial^2 T}{\partial t^2} \frac{\Delta t^2}{8} \right) \quad (17)$$

We will determine the truncation physics for the following discrete equation:

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} - F(\phi^n, \phi^{n+1}, \Sigma_f^n, \Sigma_f^{n+1}) = 0 \quad (18)$$

For operator split coupling we have

$$F(\phi^n, \phi^{n+1}, \Sigma_f^n, \Sigma_f^{n+1}) = \phi^n \Sigma_f^n \quad (19)$$

Here the cross section and flux are evaluated at the old time level because that is the only way to make $\phi \Sigma_f$ consistent in Eq. (4) and (5) without iteration. For the fully implicit coupling we have

$$F(\phi^n, \phi^{n+1}, \Sigma_f^n, \Sigma_f^{n+1}) = \phi^{n+1} \Sigma_f^{n+1} \quad (20)$$

Here some form of nonlinear iteration is required to put both terms at new time simultaneously. This iteration increases the cost of the fully implicit approach. Finally we have the second order approach

$$F(\phi^n,\phi^{n+1},\Sigma_f^n,\Sigma_f^{n+1})=\frac{1}{2}\left(\phi^{n+1}\Sigma_f^{n+1}+\phi^n\Sigma_f^n\right) \quad (21)$$

This is the Crank-Nicolson method. For the operator split coupling we substitute Eq. (9), Eq. (15), and Eq. (19) into Eq. (18). Combining terms results in

$$\begin{aligned}&\left(\frac{\partial\phi}{\partial t}-\frac{\Delta t}{2}\frac{\partial^2\phi}{\partial t^2}\right)\\&-\left(\phi-\frac{\partial\phi}{\partial t}\Delta t\right)\left(\Sigma_f-\frac{\partial\Sigma_f}{\partial T}\frac{\partial T}{\partial t}\Delta t\right)=O\left(\Delta t^2\right)\end{aligned} \quad (22)$$

Here we see that the transient neutron flux has been modified by the addition of a nonphysical temporal diffusion operator. The neutron flux has a physical component and a nonphysical component that scales like the time derivative of the flux. The fission cross section has been modified by a nonphysical component that scales like the derivative of the cross section with respect to time (set by the fuel) and the derivative of temperature with respect to time (set by the transient). It is important to note here that the unphysical truncation physics all scale with Δt and they all go to zero in steady state since they all contain either first or second order derivatives with respect to time. These errors impact the transient, not the steady state.

Second consider the fully implicit coupling. Here we substitute Eq. (9), and Eq. (20) into Eq. (18). Combining terms yields

$$\left(\frac{\partial\phi}{\partial t}+\frac{\Delta t}{2}\frac{\partial^2\phi}{\partial t^2}\right)-\phi\Sigma_f=O\left(\Delta t^2\right) \quad (23)$$

One notices that the form of the transient neutron flux is identical between the operator split coupling and the fully implicit coupling. The main difference is the source term errors are removed. And finally consider the 2nd order in time coupling. Here we substitute Eq. (10), Eq. (11), Eq. (16), Eq. (17), and Eq. (21) into Eq. (18). Combining terms results in

$$\begin{aligned}&\left(\frac{\partial\phi}{\partial t}+\frac{\Delta t^2}{24}\frac{\partial^3\phi}{\partial t^3}\right)\\&-\left(\phi+\frac{\partial^2\phi}{\partial t^2}\frac{\Delta t^2}{8}\right)\left(\Sigma_f+\frac{\partial\Sigma_f}{\partial T}\frac{\partial^2 T}{\partial t^2}\frac{\Delta t^2}{8}\right)=O\left(\Delta t^3\right)\end{aligned} \quad (24)$$

Here the transient truncation term is dispersive in time and the flux and cross section truncation term is diffusive in time. All of these truncation physics terms disappear in steady state and scale with Δt^2.

Additional study of the details of this process is certainly required but initial findings indicate the following. The operator split method seems to amplify small changes. Power transients are more violent because the feedback mechanisms are under predicted. Fully implicit over damps the oscillations making the transients more stable than is physically correct. The error for both first order methods is different but the scale the same. So with operator split you have less stability and inaccuracy and for fully implicit you have more stability and inaccuracy.

It should be noted that for steady state calculations the stability afforded by the additional damping may be a real benefit to speed without affecting that accuracy of the steady state solution (note all truncation errors are zero in steady state). However, if one is looking for accurate transient results from a fully implicit approach, even through the code will be stable for large times steps, small time step may be required to keep the truncation physics from impacting the solution.

From the second order solution one can see that all of the truncation physics terms that scale with Δt are gone. There are still truncation physics, but since they scale like Δt^2 their impact on the solution is minimal. There are drawbacks to both first order methods but if possible it is best to simply use a method that is second order accurate.

It is important to note here that if the neutronics code and thermal hydraulics code are developed separately, that the truncation error discussed in this section are not a part of either code. One could verify and validate the neutronics and thermal hydraulics code separately and "prove" their accuracy. But this error comes from the coupling of the two codes which is not addressed in the verification and validation of either code independently. For coupled calculations the components need to be first verified and validated separately and then re-verified and re-validated as a system.

4. Results

The first step in the results is to show accuracy. The above discussion of truncation physics was highly simplified, so it is important to verify that the second order solution method is second order accurate in time. The solution method used in the Physics-based preconditioned Jacobian-free Newton-Krylov method. The transient is initiated by turning off the pump shown in Fig. 1. A series of transients were run with both a first and second order accurate in time method. The error is computed from the following equation

$$\text{Error} = \left[\Sigma(\text{computed} - \text{base})^2\right]^{1/2} \qquad (25)$$

The base solution is computed from the second order method with a time step ten times smaller than the smallest on the plot. This results in a solution one hundred times more accurate. The accuracy of the results was then computed and is shown in Fig. 2.

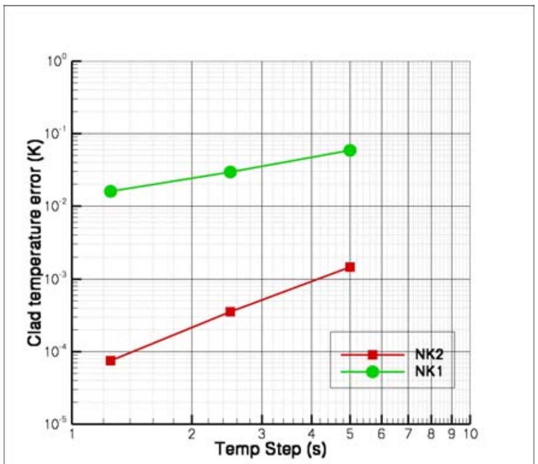

Fig. 2 Time step convergence plot.

In Fig. 2 we see the first order error shown in green and the second order error shown in red. The slope of the first order error is one and the slope of second order error is two. The second order error is clearly much smaller than the first order error. Because the slope of the second order method is two this clearly indicates that there are no truncation physics that scale with Δt.

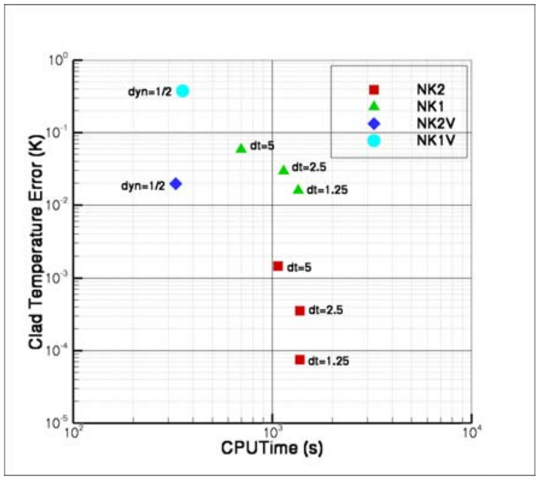

Fig. 3 Efficacy plot.

Fig. 3 shows an efficacy plot (error vs. CPU time). This plot very quickly answers two questions, “For a set amount of error how much CPU time is required?” This is a horizontal line on the diagram. The second question is, “For a set amount of CPU time how much error is there?” This is answered by a vertical line. In general one wants to be in the lower left hand corner of the plot, low error and low CPU time.

This plot shows that there is a significant difference in accuracy between the first (green triangles) and second (red squares) order accurate methods. It also shows two new data points not shown in Fig. 2. The dark blue diamond is the second order method run with a variable time step and the light blue circle is the first order method run with a variable time step (the previous 1st and 2nd order methods are run with constant time steps).

The second order method can be run with a larger time step and still maintain the same accuracy as the first order method. However, one notices that when the first order method is run with large time steps the first order truncation physics have a negative impact on accuracy. So, due to the increased stability the fully implicit 1st order method can run at large time steps, however if one is interested in the accuracy of the transient, small time steps still have to be taken. There is a significant difference between stability and accuracy. However, if one is simply looking for a steady state solution without interest in the accuracy of the transient, the fully implicit first order method is an ideal candidate.

Figure 4 shows the results from the unprotected loss of flow (ULOF) transient. Here we see the initial power drop caused by the heating of the fuel which results from the lower heat removal caused by the coolant flow slowing down due to the transition from forced convection to natural circulation when the pump is turned off. This takes place in the first 500 second of the transient. Due to the reduction in power during this time period, the coolant temperature lowers and the fuel temperature lowers resulting in an increase in power which peaks at about 1100 seconds. Approximately 1100 second is the maximum power in the transient and is most likely when core damage would result. For safety simulations, accurately capturing the time and height of this peak is important.

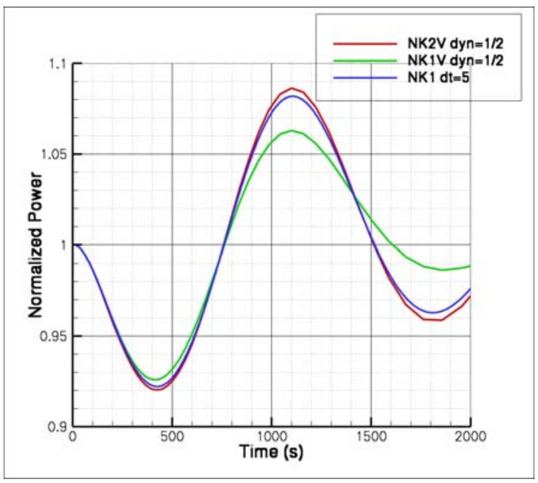

Fig. 4 Power as a function of time.

It is important to reiterate here that this model is very simple and there is no claim that these results are validated for use in any decision making process. The purpose of this manuscript is to evaluate qualitatively (not quantitatively) the impacts of numerical methods on the solution. More precisely we are focusing on the impact of numerical methods in tightly couple (no SCRAM) transients that rely on passive safety (neutronic feedback and natural circulation).

Figure 4 shows three sets of results. The second order answers are shown in red. The small time step first order method is shown in blue and the large time step first order method is shown in green. First, one can see that the first order solution and the second order solution converge to the same solution with small time steps. Second, one can see that the error in the first order method is larger when larger time steps are used. The last observation is that the error made caused by the first order truncation physics grows with time.

Here it is useful to note that at about 4000 second the reactor goes back to steady state at the same power level it was at time 0 (since the heat removal by the IHX is constant, in steady state the reactor power is a fixed value).

The first order method with large time steps under predicted the power drop at about 500 seconds. This is caused by the first order truncation physics modifying the cross sections and effectively changing the feedback control. Since the power did not go down as low as it should have, the coolant did not cool off as much. Consequently, the warmer coolant, over-predicted the feedback (due to truncation physics) for the power rise. The result is a larger under-prediction of the power rise at 1100 seconds than the under-prediction of the power drop at 500 seconds. What this shows is that the error is being compounded.

If one considers the system, the error in the cross sections causes an error in power, the error in power causes an error in flow rate by changing the buoyancy force (feedback from neutronics to fluid flow), this causes an error in the coolant temperature entering the core and the process repeats. In a closed loop under natural circulation there is no way for the error to leave the system.

The physical time scales of the transient are shown in Fig. 5. The time scales are calculated from Eq. (26). Here the physical time scale for variable θ is given as τ_θ. In Fig. 5 the time scales are broken into time step as black (implicit solid, semi-implicit dashed), coolant blue (the lower blue line is coolant velocity), neutronics in green, and thermal conduction in red.

$$\tau_\theta = \frac{1}{\left|\frac{1}{\theta}\frac{\partial \theta}{\partial t}\right|} \tag{26}$$

All physical time scales in this transient are slow. The fastest is the change in the Fluid when the pump is turned off. There is a minor change in Conduction as the core heats up and cools off but this ends in a few hundred seconds. The transient to steady state is governed by the gentle oscillations in the Neutronics as the reactor finds a new equilibrium.

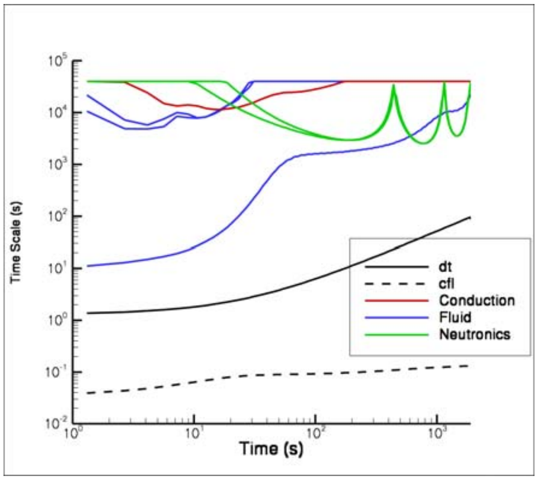

Fig. 5 Physical time scales of the transient.

There are a few important observations to make here. First, it is interesting to note that a semi-implicit method for fluid flow would be required to run at time steps around one tenth of a second even though all of the physical time scales are on the order of 1000 seconds. The approximations made in the semi-implicit method introduce truncation physics that cause the solution to become unstable above the CFL limit.

Second, it is also interesting to point out that even though this is a slow and gentle transient, numerical errors made by the time integration method can become important. Because of the coupling between the neutronics, thermal conduction, and fluid flow there are more forms of truncation physics. These three physics have very different time scales so the coupling errors can be large even when the individual errors would be small.

Figure 6 shows the peak clad temperature for this transient. Three results are shown. The black line is the second order method with a variable time step. The red dashed line (which overlays the black line) is the first order method with a small constant time step. The green line is the first order method with a variable time step. There are two observations to be made from this plot. First large changes in power may only lead to small changes in design criteria like peak clad temperature. The purpose of this manuscript is to illuminate future research to be done to quantify these effects in physically realistic and quantitatively correct simulations.

Second, it is important to note that the peak clad temperature is under predicted (non-conservative) by the first order (green line) in time method with large time steps. With multi-physics, multi-scale simulations that are tightly coupled through a variety of nonlinear feedback mechanisms one has to use caution to ensure that their safety calculations are truly conservative.

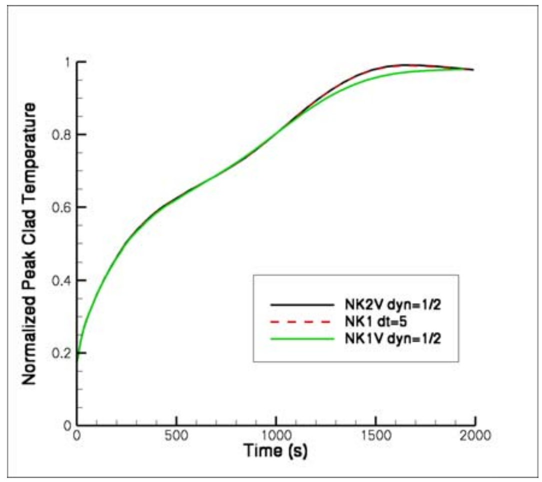

Fig. 6 Peak clad temperature.

In closing, it is worthwhile to comment on the interaction between accuracy, validation, and uncertainty quantification. Unless one is careful to ensure that the truncation physics in the simulation is small, it is possible that the validation and uncertainty quantification processes may be evaluating the truncation physics and not the physical model that they were intended to measure. This problem is exacerbated by modern passively safe reactor designs that have closed loops, with long transients, and multiple feedback mechanisms between the coupled physics. In this case it is possible for the numerical errors to cause the solution to drift away from the physical solution.

5. Conclusions and Future Work

This work is a continuation of other work on quantifying the impact of numerical accuracy on reactor safety simulations. This manuscript represents highly simplified models that are intended for qualitative illumination of possible problems. Future work will focus on bringing the reality of these simulations into the quantitative realm.

The purpose of the manuscript is to caution the reader so they are aware of possible problems that they may encounter while investigating the safety of passive reactor designs. Care should be give prior to validation and uncertainty quantification to ensure that one is measuring the physical model and not the truncation physics.

6. Acknowledgement

Prepared for the U.S. Department of Energy Office of Nuclear Energy Under DOE Idaho Operations Office Contract DE-AC07-05ID14517 (INL/CON-08-14245).

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